Supplementary Information

Table S1: Generated excited-state orbitals of (tfc)$Ir^{III}(NH_3)_2$

Symmetry of ionized orbital	Orbital number in Ir^{III}	Resulting spin density on Ir	Resulting atomic charge on Ir	Energy relative to Ir^{IV} ground state (eV)
B_1	107	-0.01	0.88	0.00
A_2	106	0.07	0.91	0.54
A_2	104	0.24	0.92	1.21
B_1	105	0.35	0.97	1.21
B_1	103	0.00	0.89	2.27
A_1	102	0.91	1.18	2.53

Table S2: Generated excited-state orbitals of (tfc)$Rh^{III}(NH_3)_2$

Symmetry	Orbital number	Spin density on Rh	Atomic charge on Rh	Relative energy (eV)
B_1	107	-0.01	0.79	0.00
A_2	106	0.02	0.81	0.63
A_2	105	0.19	0.84	1.58
B_1	104	0.22	0.85	1.62

B_1	103	0.00	0.80	2.28
A_1	99	0.77	1.05	3.19

Table S3: Generated excited-state orbitals of (tfc)$Co^{III}(NH_3)_2$

Symmetry	Orbital number	Spin density on Co	Atomic charge on Co	Relative energy (eV)
B_1	107	-0.02	0.48	0.00
A_2	106	0.00	0.49	0.67
A_2	105	0.08	0.50	1.94
B_1	104	0.10	0.50	2.02
B_1	103	-0.01	0.49	2.33
A_1	98	1.16	0.69	3.19

Table S4: Generated excited-state orbitals of (tpfc)$Ir^{III}(NH_3)_2$

Symmetry	Orbital number	Spin density on Ir	Atomic charge on Ir	Relative energy (eV)
B_1	215	-0.01	0.88	0.00
A_2	214	0.07	0.90	0.15

A_2	212	0.08	0.85	0.59
B_1	213	0.38	0.97	0.86
A_1	211	0.89	1.17	2.06

Table S5: Generated excited-state orbitals of (tpfc)$Rh^{III}(NH_3)_2$

Symmetry	Orbital number	Spin density on Rh	Atomic charge on Rh	Relative energy (eV)
B_1	215	-0.01	0.79	0.00
A_2	214	0.02	0.80	0.24
A_2	213	0.21	0.84	1.23
B_1	212	0.24	0.86	1.27
A_1	202	0.75	1.04	2.71

Table S6: Generated excited-state orbitals of (tpfc)$Co^{III}(NH_3)_2$

Symmetry	Orbital number	Spin density on Co	Atomic charge on Co	Relative energy (eV)
B_1	215	-0.02	0.47	0.00
A_2	214	0.00	0.48	0.27
A_2	213	0.10	0.48	1.63

B_1	212	0.12	0.49	1.71
A_1	201	1.13	0.66	2.74

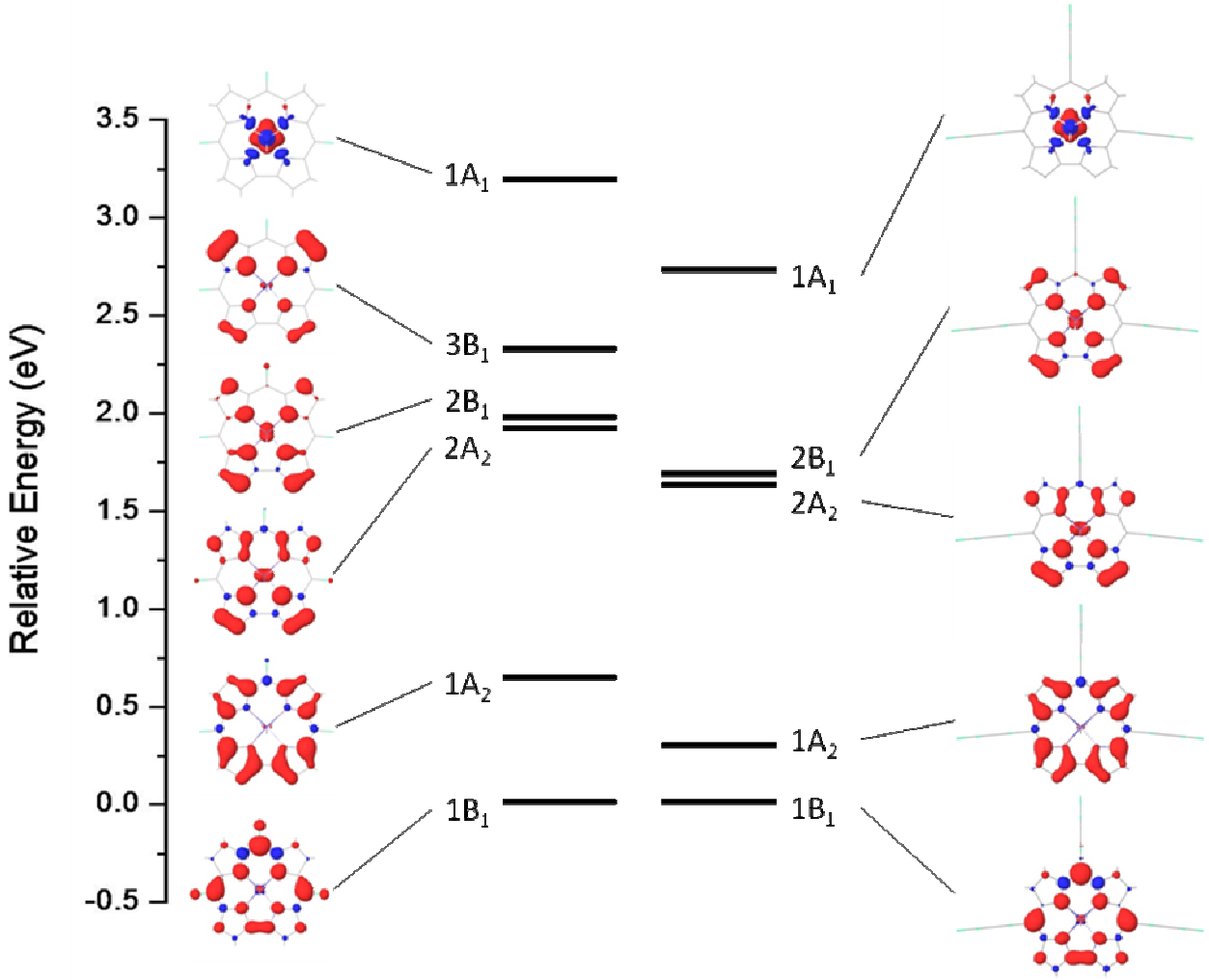

Figure S1: Orbital drawings and energies for $[(tfc)Co(NH_3)_2]^+$.

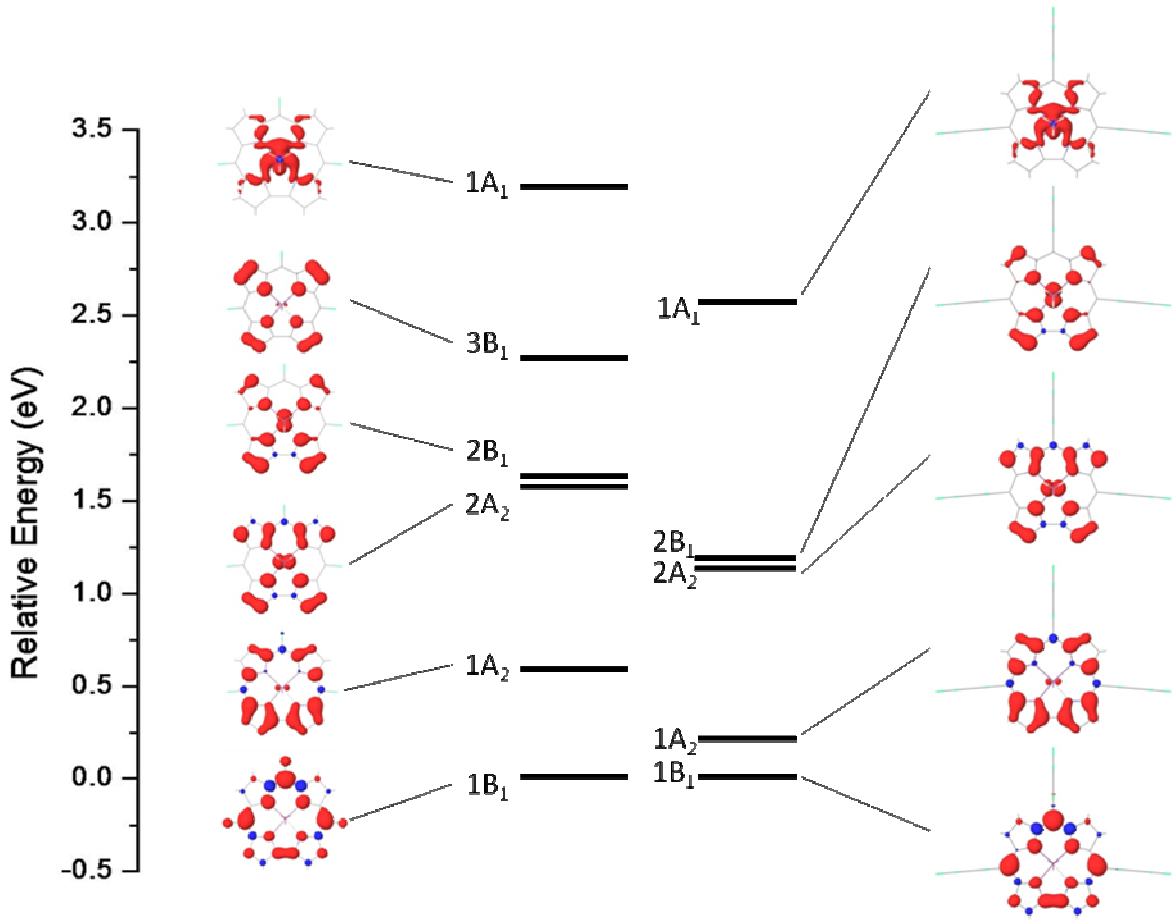

Figure S2: Orbital drawings and energies for $[(tfc)Rh(NH_3)_2]^+$.

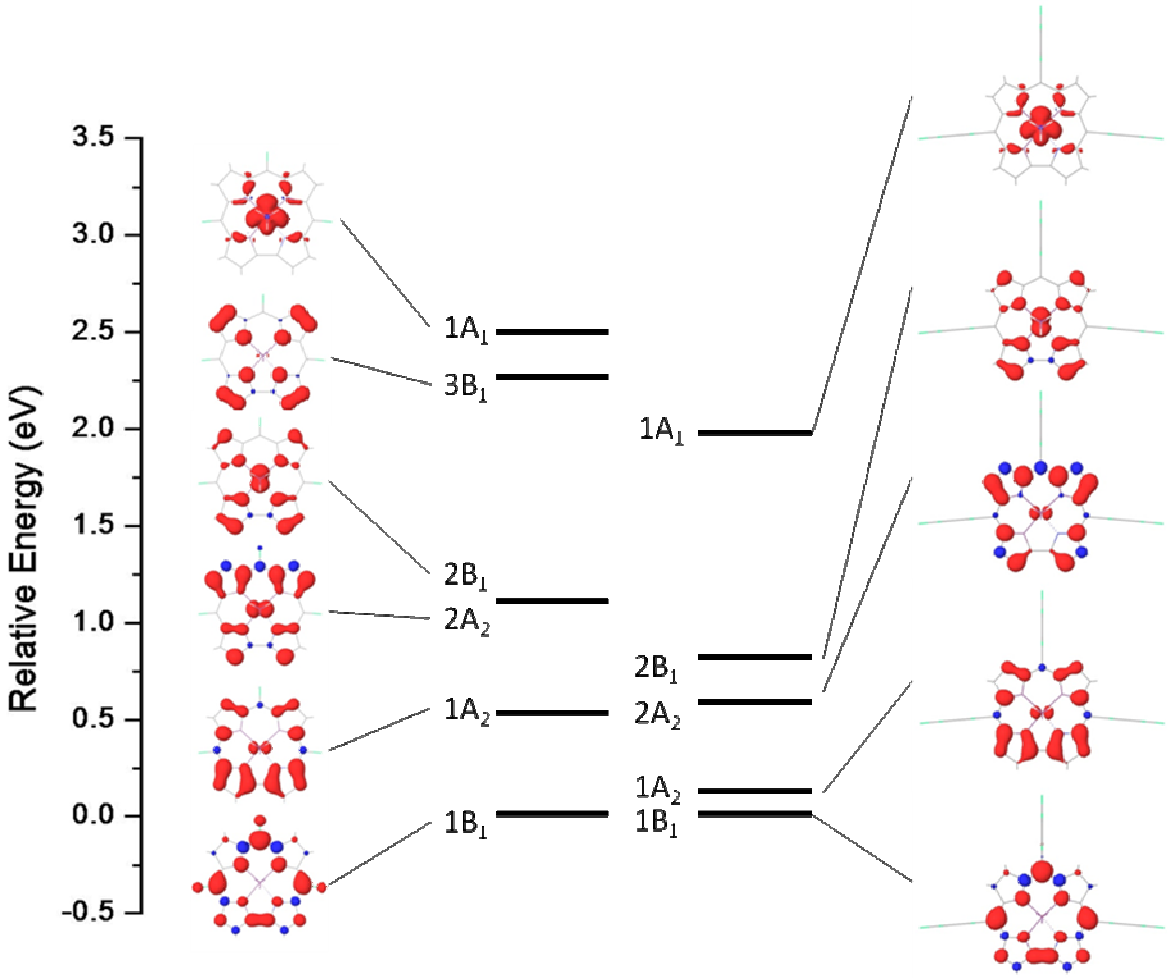

Figure S3: Orbital drawings and energies for $[(tfc)Ir(NH_3)_2]^+$.